New *α*-Ditetralonyl Glucoside from The Green Walnut Husk of *Juglans mandshurica*

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Abstract

One new *α*-ditetralonyl glucoside (**1)**, was isolated from the green walnut husk of *Juglans mandshurica* (Juglandaceae), together with twelve known compounds (**2-13**). The structure of the new compound was determined as (2*R*,4*S*,10*S*,12*S*)-2-[7-(12,13,16-trihydroxy-*α*-tetralonyl-13-*O*-*β*-D-glucopyranoside)]-4,8-dihydroxy-*α*-tetralone-4-*O*-*β*-D-glucopyranoside (**1**), on the basis of detailed spectroscopic analyses, and acidic hydrolysis. Compounds **6**, **7** and **11** were isolated from the genus *Juglans* for the first time. Compound **1-13** showed weak cytotoxic against A549 and HeLa cell lines.

Keyword

Juglans mandshurica, Juglandaceae, *α*-ditetralonyl glucoside, cytotoxic activity

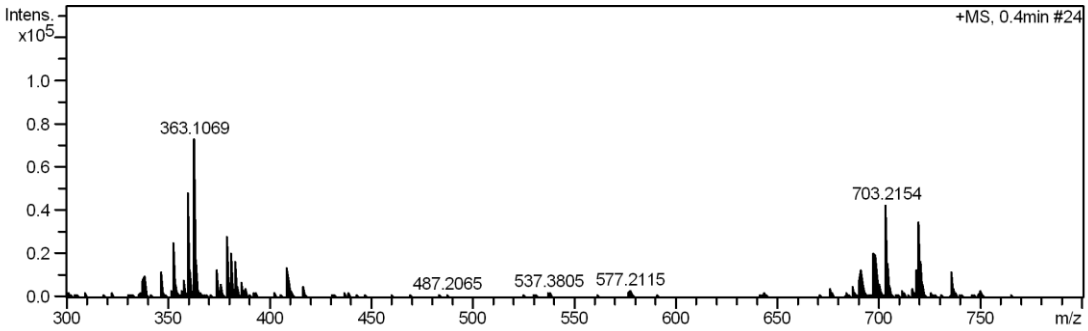

Figure S1. HR-ESI-TOF MS spectrum of compound **1**

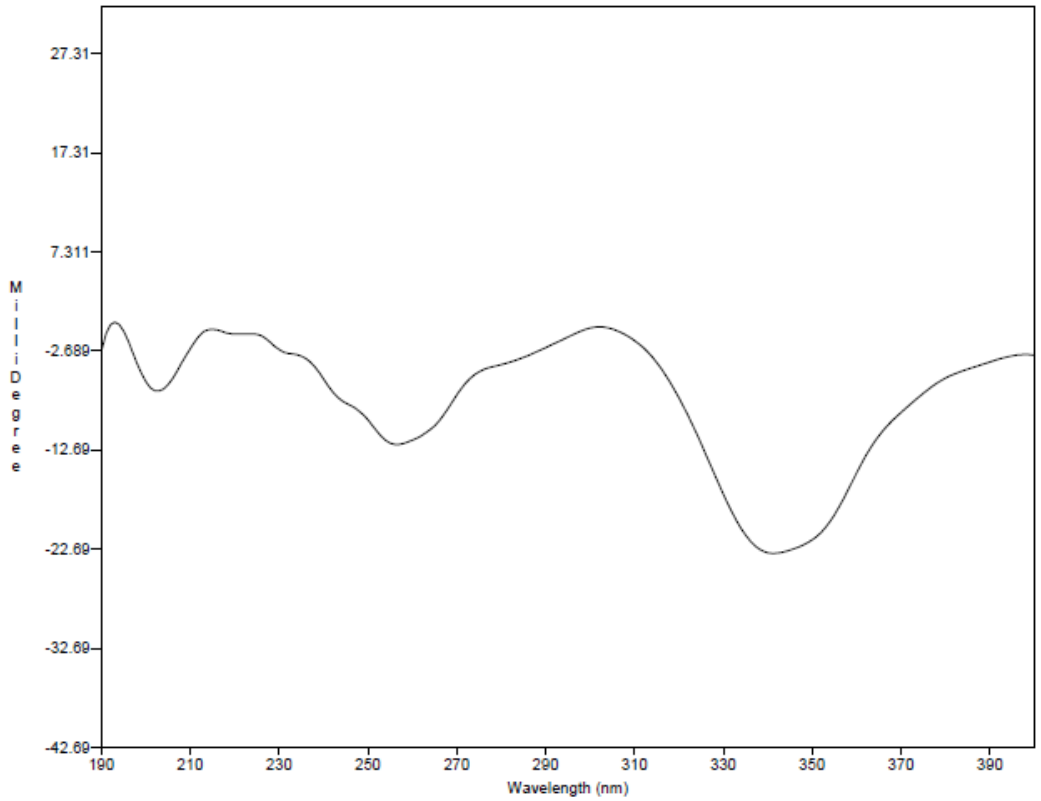

Figure S2. CD spectrum of compound **1**

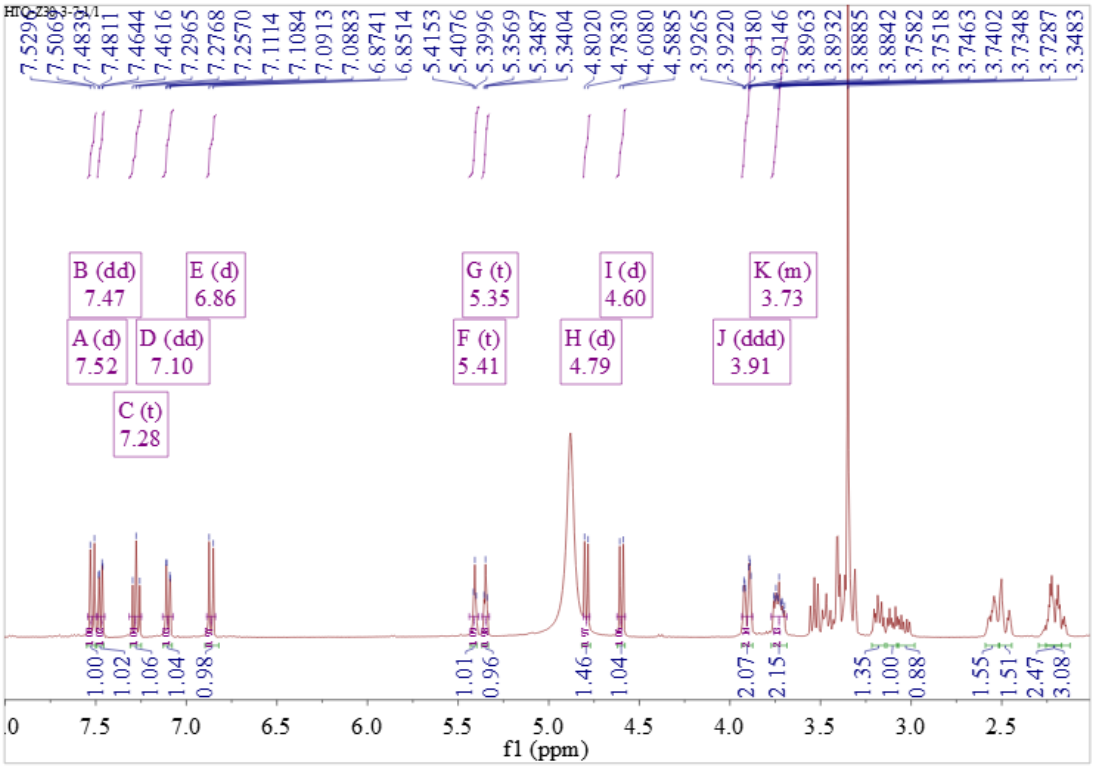

Figure S3. The ^{1}H NMR (Methanol-d_4, 600 MHz) spectrum of compound **1**

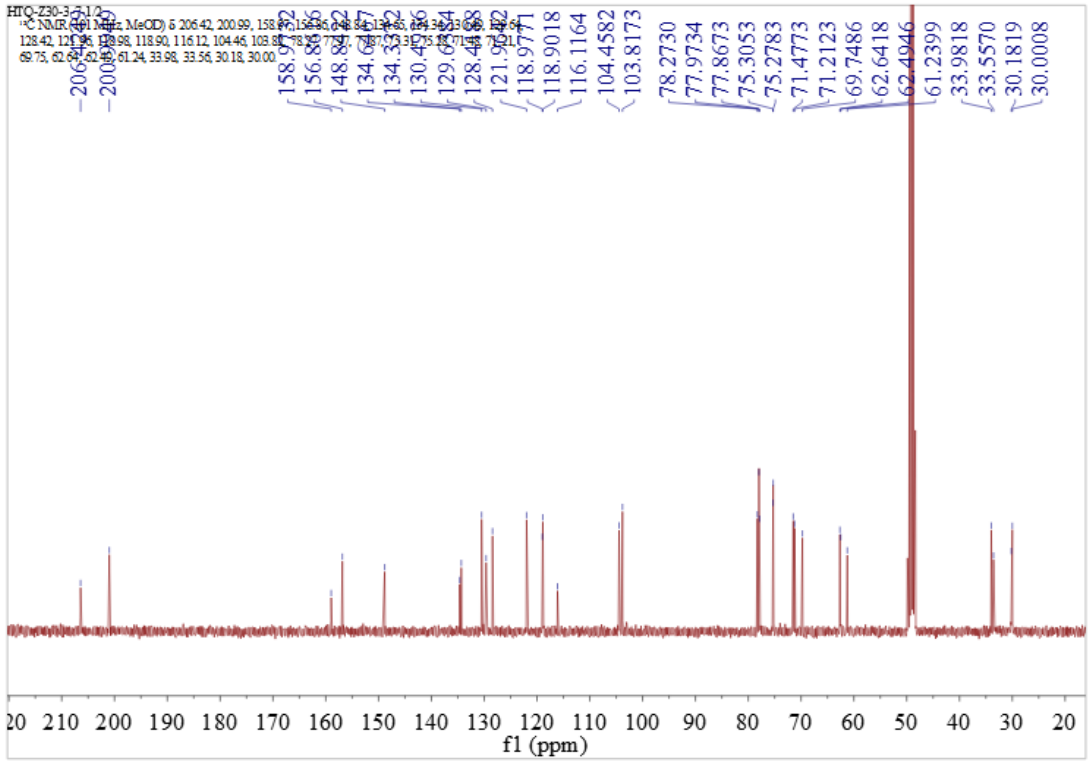

Figure S4. The ^{13}C NMR (Methanol-d_4, 100 MHz) spectrum of compound **1**

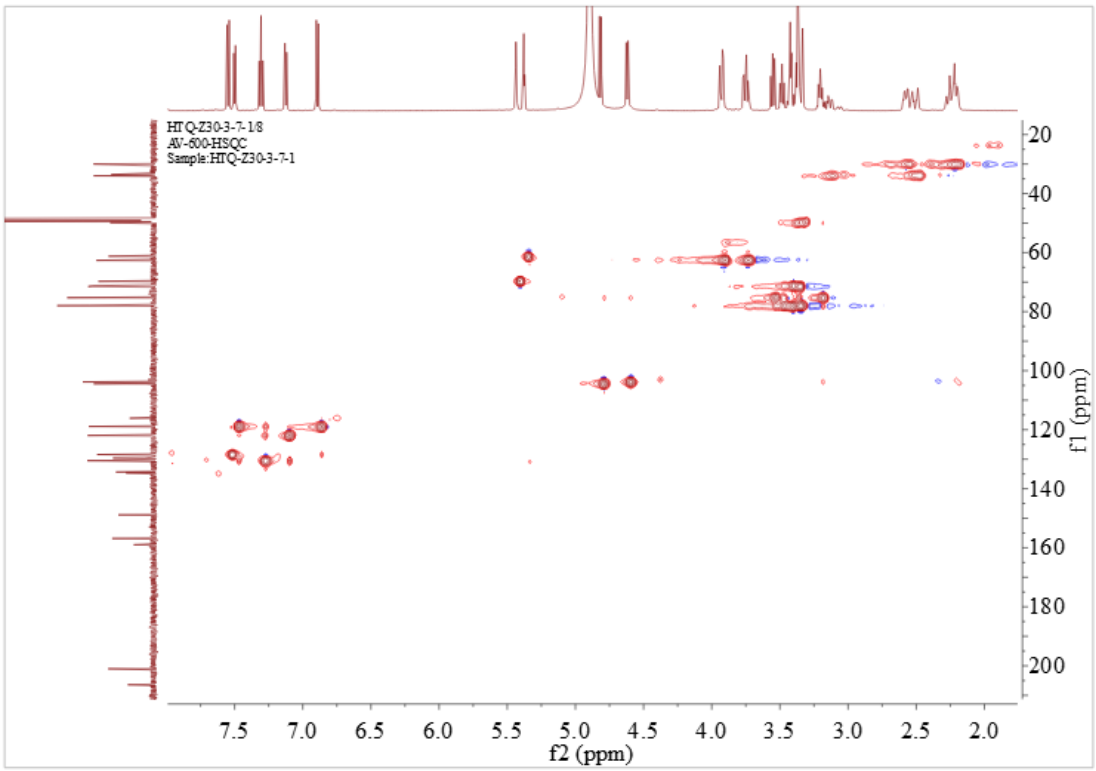

Figure S5. HSQC spectrum of compound **1**

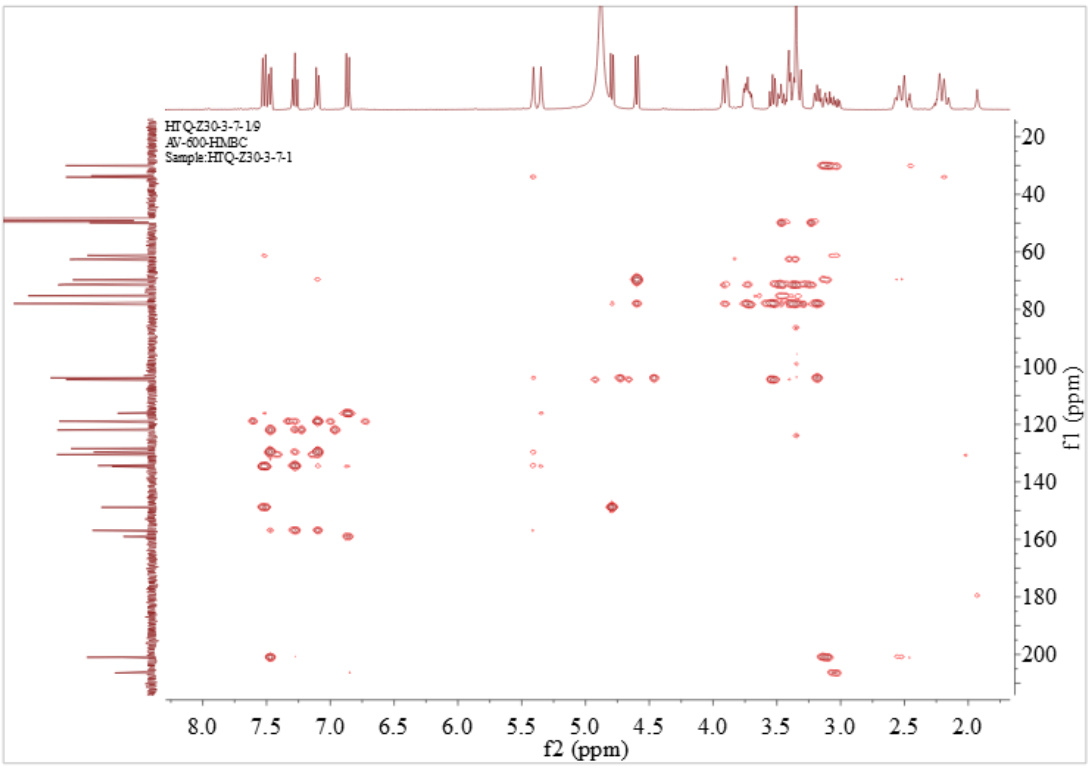

Figure S6. HMBC spectrum of compound **1**

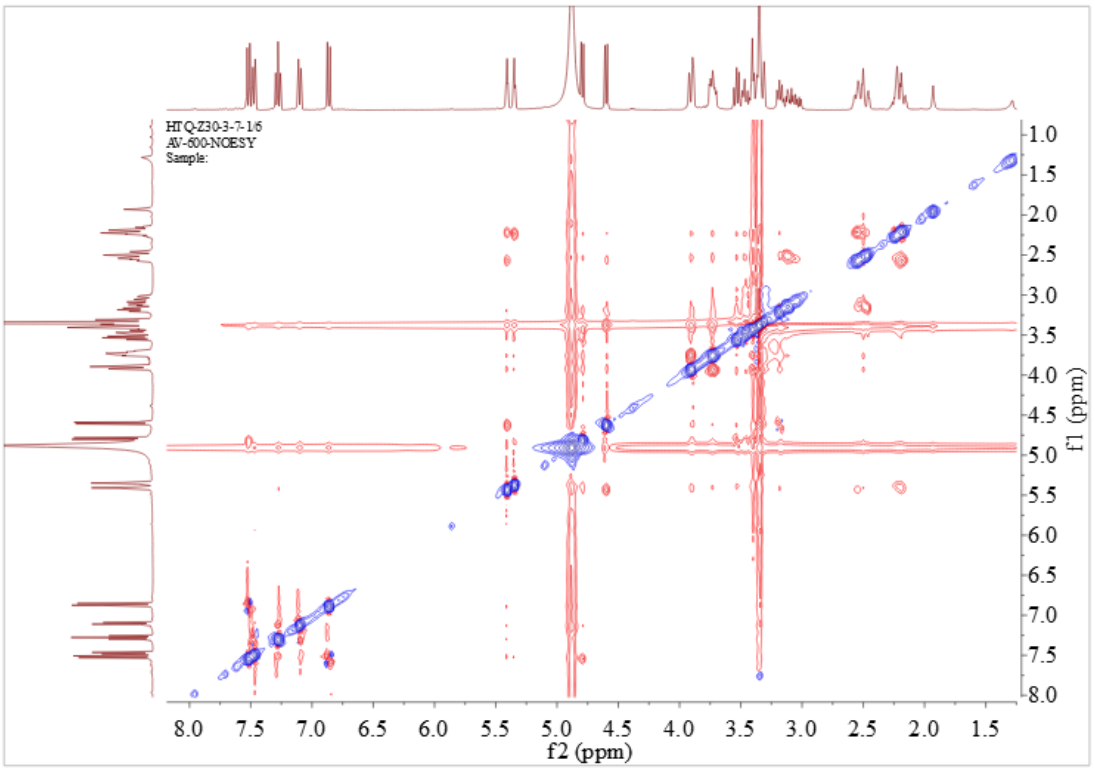

Figure S7. NOESY spectrum of compound **1**

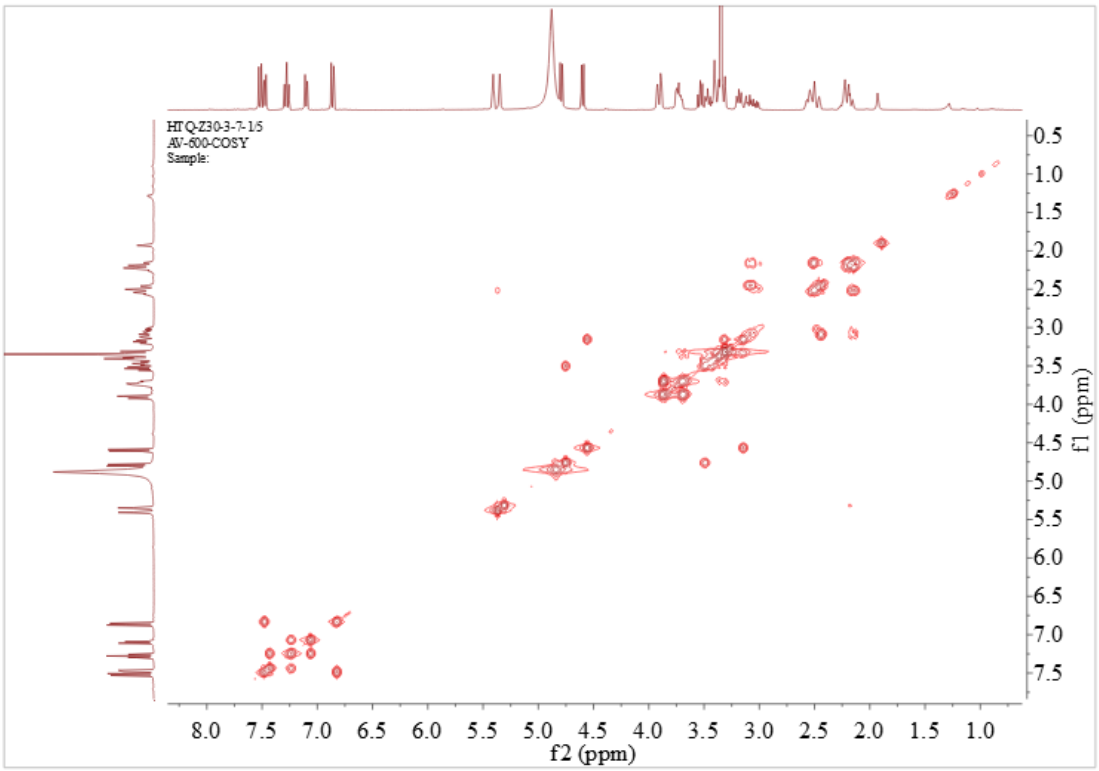

Figure S8. ^{1}H-^{1}H COSY spectrum of compound **1**

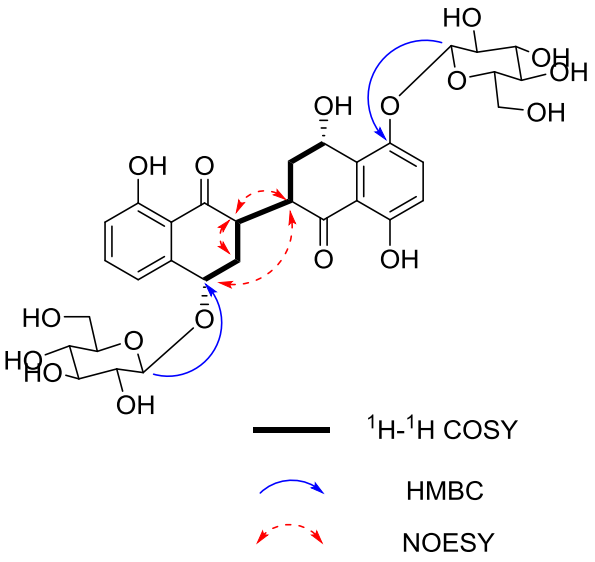

Figure S9 the key ^{1}H-^{1}H COSY, HMBC and NOESY correlations of compound **1**

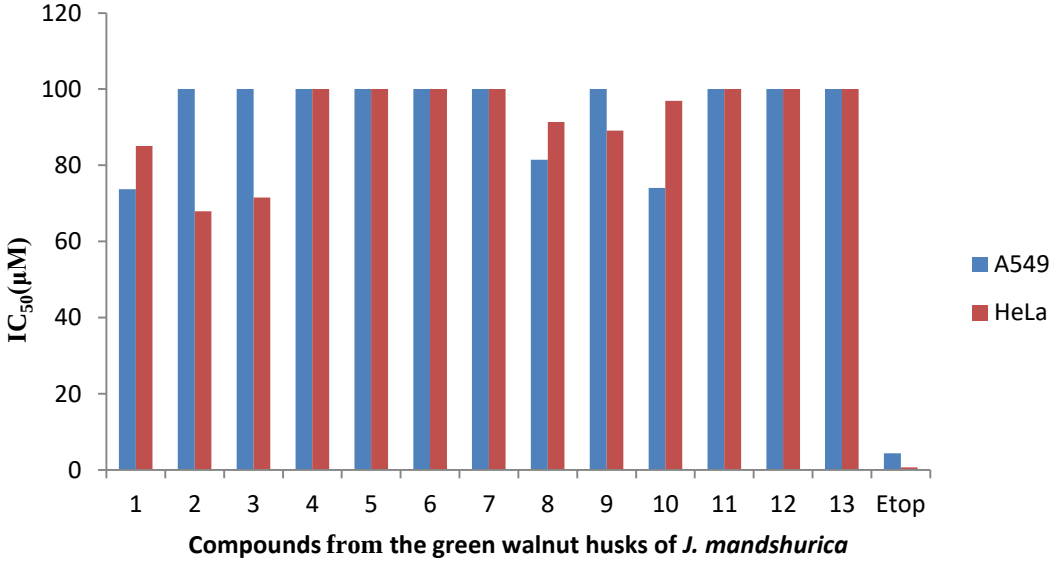

Figure S10 Cytotoxic activities of compounds against two human cancer cell lines

Table S1 Cytotoxicity data of isolated compounds **1-13.**[a]

Compound	IC_{50} (μM)		Compound	IC_{50} (μM)	
	A549	HeLa		A549	HeLa
1	73.7	85.1	**8**	81.5	91.4
2	>100	67.9	**9**	>100	89.1
3	>100	71.5	**10**	74.1	96.9
4	>100	>100	**11**	>100	>100
5	>100	>100	**12**	>100	>100
6	>100	>100	**13**	>100	>100
7	>!00	>100			
Etoposide[b]	4.4	0.7			

A549: human lung cancer cell lines

HeLa: human cervical carcinoma cancer cell lines

[a] Data expressed as IC_{50} values (μM);

[b] Positive control.